

372a Multiscale Modeling and Density of States Monte Carlo of Different Glass Formers

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The computational demand of glassy systems is prohibitively high even with the most advanced hardware. We employ two special techniques, coarse-grained molecular dynamics (CGMD) and density of states Monte Carlo (DOSMC), to better understand the properties of low molecular weight glasses as well as glassy polymers. By omitting the atomistic details and joining each monomer into one big superatom, CGMD can obtain a mesoscale model to investigate the glassy polymer relaxation behaviors at a reasonable expense. We optimize the mesoscale model until the radial distribution function generated from the mesoscale model is consistent with the one from atomistic scale. We apply this technique to the low molecular weight glass former ortho-terphenyl as well as polystyrene. Extensions of this technique to the interplay of the local chain neighborhood of Polystyrene and Polyisoprene blend at various temperatures and concentrations are currently in progress, aiming to identify what contribute to the CG mapping potentials. Still Molecular Dynamics alone is not able to equilibrate even the simplified glass models. DOSMC is an efficient technique to calculate the density of states and therewith the partition function in complex systems. We apply it to a understand a binary Lennard-Jones model glassy former and combine it with coarse graining to model ortho-terphenyl, a real glass former. Finally differences between bulk and confined systems are pointed out.